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Probability adjoint identification of airborne pollutant sources depending on few sensors in a vented room with conjugate heat and species transports

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Abstract

The definition and governing equation of probability density function (PDF) have been implemented in the present work. The procedure is applied to the backward time identification of the pollutant probability density function history and finally the maximal probability density of source location in a two-dimensional slot ventilated building enclosure with two solid blocks. Steady-state airflow field, sensor location, boundary conditions, thermo-physical properties and geometric characteristics should be known in prior. Spatial probability density function history has been computed under four ventilation modes, i.e., mixed ventilation (MV), displacement ventilation (DV), mixed ventilation with top ceiling outlet (MVS), and displacement ventilation with left side outlet (MVS). Effects of pollutant source location and alarming sensor on the accuracy of the probability density function have been conducted. Different positions of pollutant sources put great effort on the inverse pollutant source identification through probability density function distribution. The pollutant sources will be more easily identified for the concentrated pollutant strips, where pollutant diffusion is efficient compared with the pollutant source at outlet.

Particularly, the good agreement of the probability density function identified source location with the true situation fully shows that adjoint probability density function method is more competitive in the engineering applications involving with convective fluid flows.

Keywords

Probability density function; slot ventilation, CFD, pollutant dispersion, solid blocks

Main text

Nomenclature

NOMENCLATURE

B	depth of the enclosure (m)	Greek symbols	
C	dimensionless contaminant concentration	Β	Buoyancy ratio
C_μ	turbulence model constant	Ρ	density (kg/m^3)
Deff	Species turbulent diffusion coefficient	μ_{eff}	Turbulent diffusion coefficient
E	dimensionless dissipation rate	υ_t	Turbulent viscosity
fx	Probability density function	*Δ*	Convergent criterion
H	height of the enclosure (m)	Θ	Heat function
K	dimensionless turbulent kinetics	*Φ*	stream function
M	contaminant releasing mass	*Ψ**	Dimensionless probability density function
M1	contaminant in unit volume	*δ*	impulse function
P	dimensionless pressure		
Re	Reynolds number	***Subscripts***	
Sc	Schmidt number	*averg*	Average
T	dimensionless time	*C*	Central point
Ui	dimensionless velocity components	O	Outlet
W	width of the enclosure (m)	*ref*	reference
φ	general variable		
Xi	Dimensionless Cartesian coordinates		

1. Introduction

The safety of ventilation has been raised as a special concern since 911 terrorist attacks and recent respiratory syndromes (such as SARS, influenza A virus H1N1), which directly taught human beings the risk and vulnerability of building air environment. Global energy crisis and carbon emission control will on the other hand push the reduction of building energy consumed in the branches of ventilation and air conditioning, and thus the strengthened tightness of building spaces avoidably increase the vulnerability of the indoor air environment (Liu et al. 2010).

To enhance the safety of built air environment, profound knowledge and understanding of room air motions and pollutant dispersions are essentially required. As early as 1970s' computational fluid dynamics introduced into the fields of building environment, avalanche researches have been conducted, in which efficient and flexible numerical modeling and methodologies on room airflow, thermal and pollutant dispersions have been widely adopted for many sorts of investigations on the building air environment. Generally, these researches could provide the spatial distributions and temporal evolutions of room air velocities, temperature, moisture and species concentration by the prior knowledge of room air flow boundary constrains, initial distributions, and emission sources (Zhao et al. 2008, Liu et al. 2008, Chen 2009, Chen et al. 2010, Li and Nielsen 2011)6.

In many situations, initial pollutant emission and contaminant source information is usually prior unknown. Referring to the up-to-date safety problems of indoor air environment, the 'spying-covered' pollutant sources effusing un-colorful and non-scent pollutants will pose a great danger to the occupants, whom could not easily identify those pollutant sources due to their productions or emissions are essentially of no noise, no color and no scent. As a direct solution scheme, pollutant sensors should be installed to detect any chemical or biological agents or infectious viruses, to avoid occupants any possible expose to the fatal contaminant or virus. However, these pollutant sensors for detecting infectious viruses and agents are relatively expensive and bulky, such that dense distributions and deployments of these sensors in the whole building spaces are impossible (Liu and Zhai 2007). Therefore, we should identify these fatal contaminant sources merely depending on the limited information obtained from the sparsely distributed sensors.

Extensive literature reviews have shown that there were generally three categories of methodologies developed to inversely identify indoor airborne pollutant source locations and pollutant releasing history depending on the limited data from sensors. One is the backward time simulation method and it starts from the present status to identify the ever evolutions of contaminants and temporary history of dispersions (Zhang and Chen 2007a, Liu et al. 2012). In the backward time simulation process, minus time steps should be imposed, such that the history identification calculations become unstable, such that a quasi-reversibility operator should be adopted to implement the backward time simulations. Pollutant history together with source emission fluxes then can be recovered step by step backward in time. Very recently, Liu et al. (2012a) have applied the quasi reversibility formulations containing diffusion and convection terms to identify multiple pollutant sources within the slot vented rooms. The second is 'trial–error' method and it conducts forward heat, airflow and contaminant transport simulations with presumed source conditions. The assumed source parameters are then adjusted according to the difference between simulated and measured results. Conjugate gradient method is the most popular 'trial-error' method, which can accurately calculate unknown conditions with an effective parameter-adjusting algorithm. (Liu et al 2010, Liu et al 2012a, Liu et al 2012b)

The third is probability method, which however focuses on the estimate of the probability associated with a certain event. (Liu and Zhai 2008, Zhang and Chen 2007b, Liu and Zhai 2008, Liu and Zhai 2009a, Liu and Zhai 2009b). Pollutant information can be identified by maximizing or minimizing the probability density function.

In the present work, probability adjoint method will be adopted to identification of airborne pollutant sources depending on few sensors in a vented room with conjugate heat and species transports.

2. Forward pollutant transportation in the ventilated room

2.1 Physical model

As shown in Fig. 1, a slot-ventilated enclosure is attached with the bottom supplying vent and top exhaust port of same size dport respectively on the left and right sides. The rectangular enclosure is of width W and height H, and the Cartesian coordinates (x,y), with the corresponding velocity components (u,v), are indicated herein. It is assumed that the third dimension of the enclosure is large enough such that room air and heat transports are two dimensional. Six pollutant sensors have been arranged in this room, which including S1, S2, S3, S4, S_O (outlet) and S_C (central) for pollutant concentration detecting and alarming purpose.

A discrete heat source is centrally positioned on the floor. With the upward thermal buoyancy effect, the external forced convection will expectedly be aided with the thermal buoyant flows, where the displacement ventilation mode will be established. Two solid blocks A and B are located symmetric with the central line. In addition, pollutant sources of same size with unknown locations were occurred in the ventilated room.

The radiation heat transfer, viscous heat dissipation and compressibility effects are considered to be negligible. The fluid mixture (base fluid and pollutant) is modeled as a Newtonian fluid with constant density and viscosity. The effect of the density variation causing the thermal buoyancy force is taken into account through the Boussinesq approximation. Other thermo-physical properties of the fluid mixture are assumed to be independent of temperature. The mass diffusivity for the diffusion of pollutant through the mixture is also treated as constant. In the present work, fluid convection driven by the pollutant concentration difference has been omitted; that is to say, the gaseous pollutant will be passively transported by the coupled external flow and thermal driven flow.

In the general situations of air flows within the building enclosure, it is assumed that an incompressible flow of a Newtonian fluid with nearly constant density and viscosity fills the cavity. Due to the Coanda effect, this design should allow to the issuing confined wall jet to adhere, as far as possible, to the bottom and to entrain the air in the whole enclosure. The descriptions of air flow development are based on the conservative laws of mass, momentum and pollutant species, can be written as (Partankar 1980),

$$\nabla \cdot (\rho \vec{v}) = 0 \tag{1}$$

$$\frac{\partial(\rho u_i)}{\partial \tau} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = \frac{\partial}{\partial x_j}((\mu + \mu_t)\frac{\partial u_i}{\partial x_j}) + \frac{\partial}{\partial x_j}((\mu + \mu_t)\frac{\partial u_j}{\partial x_i}) - \frac{\partial p}{\partial x_i} + \rho \beta_T g_i (T - T_0) \tag{2}$$

$$\frac{\partial(\rho k)}{\partial \tau} + \frac{\partial(\rho k u_j)}{\partial x_j} = \frac{\partial}{\partial x_j}((\mu + \frac{\mu_t}{\sigma_k})\frac{\partial k}{\partial x_j}) + G_k + G_b - \rho\varepsilon \tag{3}$$

$$\frac{\partial(\rho \varepsilon)}{\partial \tau} + \frac{\partial(\rho \varepsilon u_j)}{\partial x_j} = \frac{\partial}{\partial x_j}((\mu + \frac{\mu_t}{\sigma_\varepsilon})\frac{\partial \varepsilon}{\partial x_j}) + C_{1\varepsilon}\frac{\varepsilon}{k}G_k + C_{1\varepsilon}C_{3\varepsilon}\frac{\varepsilon}{k}G_b - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} \tag{4}$$

$$\frac{\partial(\rho^F \varphi_i)}{\partial \tau} + \nabla \cdot (\rho^F \vec{v} \varphi_i) = \nabla \cdot (((\rho D_{i,m})^F + \frac{\mu_t}{Sc_t})\nabla \varphi_i) \quad \text{for fluid regions} \tag{5}$$

$$\frac{\partial(\rho^S \varphi_i)}{\partial \tau} = \nabla \cdot ((\rho D_{i,m})^S)\nabla \varphi_i) \quad \text{for solid regions} \tag{6}$$

The standard *k*–*ε* model is a semi-empirical model based on model transport equations for the turbulence kinetic energy (*k*) and its dissipation rate (*ε*). The model transport equation for *k* is derived from the exact equation, while the model transport equation for *ε* was obtained using physical reasoning and bears little resemblance to its mathematically exact counterpart (Launder and Spalding 1974). In the derivation of the *k*–*ε* model, it was assumed that the flow is fully turbulent, and the effects of molecular viscosity are negligible. The standard *k*–*ε* model is therefore valid only for fully turbulent flows.

The turbulence kinetic energy and its rate of dissipation are obtained from the above transport equations. In these equations, G_k represents the generation of turbulence kinetic energy due to the mean velocity gradients, calculated as,

$$G_k = -\rho \overline{u_i' u_j'} \frac{\partial u_j}{\partial x_i} \tag{7}$$

To evaluate G_k in a manner consistent with the Boussinesq assumptions, it can be further written as,

$$G_k = \mu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \frac{\partial u_i}{\partial x_j} \tag{8}$$

Term G_b is the generation of turbulence kinetic energy due to buoyancy, and it is given by,

$$G_b = \beta g_i \frac{\mu_t}{\mathrm{Pr}_t} \frac{\partial T}{\partial x_i} \tag{9}$$

Where Pr_t is the turbulent Prandtl number for energy and g_i is the component of the gravitational vector in the *i*th direction. For the standard *k*–*ε* model, the value of Pr_t is 0.85. The coefficient of thermal expansion, β_T, is defined as,

$$\beta_T = -\frac{1}{\rho} \left(\frac{\partial \rho}{\partial T}\right)_p \tag{10}$$

It can be seen from the transport equations for *k* that turbulence kinetic energy tends to be augmented ($G_b>0$) in unstable stratification. For stable stratification, buoyancy tends to suppress the turbulence ($G_b<0$). Usually, the effects of buoyancy on the generation of *k* are always included when you have both a non-zero gravity field and a non-zero temperature (or density) gradient. While the buoyancy effects on the generation of k are relatively well understood, the effect on *ε* is less clear. In the present work, the buoyancy effects on ε are neglected simply by setting G_b to zero in the transport equation for ε (or, constant $C_{3\varepsilon}$ is setting to zero).

The turbulent (or eddy) viscosity, μ_t, is computed by combining k and ε as follows,

$$\mu_t = \rho C_\mu k^2/\varepsilon \tag{11}$$

Model constants C_μ, $C_{1\varepsilon}$ and $C_{2\varepsilon}$, and turbulent Prandtl numbers σ_k and σ_ε respectively for k and ε model have the following values (Launder and Spalding 1974),

$C_\mu = 0.09$, $C_{1\varepsilon} = 1.44$, $C_{2\varepsilon} = 1.92$, $\sigma_k = 1.00$, $\sigma_\varepsilon = 1.30$

Conjugate convective and conductive heat transfer

Building blocks are completely saturated by ambient air, and heat transfer occurs in fluid (air) region and building blocks simultaneously, i.e., combination of heat convection and heat diffusion. For fluid regions,

$$\frac{\partial((\rho C_p)^F T)}{\partial \tau} + \nabla \cdot (\vec{v}(\rho C_p)^F T) = \nabla \cdot ((\lambda^F + \lambda_t)\nabla T) + Q^F \quad \text{for fluid regions} \tag{12}$$

The effective conductivity can be defined as $\lambda_{eff} = (\lambda^F + \lambda_t)$, and λ_t is the turbulent thermal conductivity, defined according to the turbulence model being used. Due to the standard k–ε model is adopted here, $\lambda_t = C_p \mu_t/\sigma_T$ (Launder and Spalding 1974), where C_p is the specific heat of the fluid. Model constant $\sigma_T = 0.90$ is maintained.

Source term Q^F includes the heat of chemical reaction, solar radiation and any other volumetric heat sources defined in this work. Detailed radiation heat transfer model will be presented later.

$$\frac{\partial((\rho C_p)^S T)}{\partial \tau} = \nabla \cdot (\lambda^S \nabla T) + Q^S \quad \text{for solid regions} \tag{13}$$

The terms on the right hand side of the above equation are the heat flux due to conduction and volumetric heat sources within the solid, respectively.

2.2 Non-dimensional expressions

Recognizing that the convection term must maintain balance and considering the ranges of governing parameters, following dimensionless variables are adopted,

$X_i = x_i/H_{ref}$, $\boldsymbol{U}_i = \boldsymbol{u}_i/u_{ref}$, $\tau^* = \tau/(H/u_{ref})$, $K = k/u_{ref}^2$, $E = \varepsilon H/u_{ref}^3$ (14a)

$P = p/\rho u_{ref}^2$, $\theta = (T - T_{ref})/\Delta T$, $S = (s - s_{ref})/\Delta s$ (14b)

The corresponding Reynolds number is defined as,

$$Re = \rho u_{ref} H_{ref}/\mu \quad (15)$$

Where enclosure height H and velocity of right inlet u_R are utilized for length scale and velocity scale respectively. Usually, H = 2.0 m is set in the present work. In the numerical work, the Reynolds number is in a range of 10^2 to 10^6, and the air kinetic viscosity is 1.5×10^{-5} m2/s resulting in velocity of right inlet varies from 7.5×10^{-4} m/s to 7.5 m/s.

Then the governing equations can be obtained,

$$\frac{\partial U_i}{\partial X_i} = 0 \quad (16)$$

$$\frac{\partial U_i U_j}{\partial X_j} = -\frac{\partial P}{\partial X_i} + \frac{\partial}{\partial X_j}(\chi_U \frac{\partial U_i}{\partial X_j}) + \frac{\partial}{\partial X_j}(\chi_U \frac{\partial U_j}{\partial X_i}) + Ar_i \theta_i \quad (17)$$

$$\frac{\partial K U_j}{\partial X_j} + (\frac{E}{K})K = \frac{\partial}{\partial X_j}(\chi_K \frac{\partial K}{\partial X_j}) + C_\mu \frac{K^2}{E}(\frac{\partial U_i}{\partial X_j} + \frac{\partial U_j}{\partial X_i})\frac{\partial U_i}{\partial X_j} + Ar_i \frac{C_\mu \frac{K^2}{E}}{\mathrm{Pr}_t} \frac{\partial \theta}{\partial X_i} \quad (18)$$

$$\frac{\partial EU_j}{\partial X_j} + (\frac{C_{2\varepsilon}E}{K})E = \frac{\partial}{\partial X_j}(\chi_E \frac{\partial E}{\partial X_j}) + C_{1\varepsilon}C_\mu K(\frac{\partial U_i}{\partial X_j} + \frac{\partial U_j}{\partial X_i})\frac{\partial U_i}{\partial X_j} + C_{1\varepsilon}C_{3\varepsilon}Ar_i \frac{C_\mu \frac{K^2}{E}}{\Pr_t}\frac{\partial \theta}{\partial X_i}$$

(19)

$$\frac{\partial \theta U_j}{\partial X_j} = \frac{\partial}{\partial X_j}(\chi_\theta \frac{\partial \theta}{\partial X_j}) \text{ in fluid domain} \tag{20}$$

$$0 = \frac{\partial}{\partial X_j}((\frac{\lambda^S}{\lambda^F}\frac{1}{\Pr \mathrm{Re}})\frac{\partial \theta}{\partial X_j}) \text{ in solid domain} \tag{21}$$

$$\frac{\partial \varphi^*}{\partial \tau^*} + \frac{\partial \varphi^* U_j}{\partial X_j} = \frac{\partial}{\partial X_j}((\frac{1}{Sc\,\mathrm{Re}} + \frac{C_\mu \frac{K^2}{E}}{Sc_t})\frac{\partial \varphi^*}{\partial X_j}) \tag{22}$$

$$\left(\frac{\rho^S}{\rho^F}\right)\frac{\partial \varphi^*}{\partial \tau^*} = \frac{\partial}{\partial X_j}((\frac{(\rho D)^S}{(\rho D)^F}\frac{1}{Sc\,\mathrm{Re}})\frac{\partial \varphi^*}{\partial X_j}) \tag{23}$$

$$Re = \rho u_{ref} H_{ref}/\mu,\ \mathrm{Ar} = \beta g H_{ref} \triangle T/u_{ref}^2,\ Sc = \mu/\rho D \tag{24}$$

$$\Theta = (T - T_{ref})/\triangle T,\ \varphi^* = (\varphi - \varphi_{ref})/\triangle\varphi \tag{25}$$

Tests were conducted for all the applications to determine the dependency of solutions upon grid size. Solutions were obtained with successive refinement of grid size, i.e., reduction in the spacing between grid nodes in the x and y directions. When solutions were observed to be unaffected by further refinements, they were presumed to be grid independent.

2.3 Species transport equations

Conservation equations for chemical species should be solved, and the local mass fraction of each species, φ_i, should be predicted through the solution of a convection-diffusion equation for the ith species. This conservation equation takes the following general form, Where Sc_t is the turbulent Schmidt number, and $Sc_t = \mu_t/(\rho D_t)^F$, D_t is the turbulent diffusivity. Usually, Sc_t maintains the constant 0.70. Turbulent diffusion generally overwhelms laminar diffusion, and the specification of detailed laminar diffusion properties in turbulent flows is generally not warranted. Additionally, for many multi-component mixing flows, the transport of enthalpy due to species diffusion can have a significant effect on the enthalpy field and should not be neglected, particularly as the Lewis number $Le_i = \lambda^F/(\rho C_p D_{i,m})^F$ is far from unity. $D_{i,m}$ is the molecular diffusion coefficient for the pollutant i in the mixture.

$$C = (c - c_{in})/(c_{ref} - c_{in}) \tag{26}$$

$$\frac{\partial C}{\partial \tau} + \frac{\partial CU_j}{\partial X_j} = \frac{\partial}{\partial X_j}(\chi_c \frac{\partial C}{\partial X_j}) + \frac{Q_c}{Q_{ref}} \tag{27}$$

$$Q_{ref} = (c_{ref} - c_{in})u_{in}/H \tag{28}$$

The air mass from a supply opening is gradually contaminated as it is regarded proportional to the time elapsed from the pollutant source.

2.4 Boundary conditions

Inflow boundaries

The boundary layer flow conditions, the power law is adopted to simulate the inflow $\boldsymbol{u}_{in}$ velocities of the atmospheric boundary layer, and the power law is given by,

$$\boldsymbol{u}_{in}(z_1)/\boldsymbol{u}_{in}(z_{ref}) = (z_1/z_{ref})^{\alpha}$$

where, $\boldsymbol{u}_{in}(z_{ref})$ is the mean wind speed at a height z_{ref}. The exponent α is the mean wind speed exponent and is dependent on upstream terrain roughness. Values of α for different terrain categories are widely published in reference (Scruton 1981).

In all cases the inflow values of perpendicular velocity w are set to zero, while the length scale of longitudinal turbulence L(z) for natural wind at the inflow boundary is approximated from the following empirical relation,

$$L(z) = 151\times(z/10)^{\alpha}\times(z_{ref}/10) \quad (29)$$

Here, $L(z)$ denotes the length scale of the velocity components in the horizontal direction at height z. The height at which the reference velocity is measured is given by z_{ref}. The length scale distribution at inflow can be prescribed through inflow values for $\varepsilon(z)$. The relationship between $\varepsilon(z)$ and $L(z)$ is defined by the following equation,

$$\varepsilon(z) = \rho C_{\mu} k(z)^{1.5}/L(z) \quad (30)$$

The turbulence intensity $\boldsymbol{I}$(z) of natural wind at height z at inflow can also be approximated by an empirical equation, which is given by the following relation,

$$\boldsymbol{I}(z) = (6.7k_{sur})^{1/2}\boldsymbol{u}_{in}(z_{ref})/\boldsymbol{u}_{in}(z) \quad (31)$$

Here, k_{sur} is a surface roughness parameter which is a measure of the surface friction coefficient of the terrain. As the value of $k(z)$ is a measure of turbulence intensity at height z, the turbulence intensity can be simulated at inflow by specifying appropriate values for $k(z)$. The relationship between $k(z)$ and $\boldsymbol{I}(z)$ is given by,

$$k(z) = 1/2[\boldsymbol{I}(z)\boldsymbol{u}_{in}(z)]^2 \quad (32)$$

Temperature and concentration of natural wind flow will be determined from the relevant weather data.

Outflow boundaries

Zero gradient outflow boundaries are adopted for all the variables, including tangential velocities, turbulent kinetics and its dissipation rate, temperature and concentrations.

Solid boundaries

Both normal and tangential velocity values are set to zero at solid boundaries. The boundary conditions for turbulence properties near solid walls are, however, more difficult to prescribe. The standard *k*–*ε* model is only valid for fully turbulent flows. A problem therefore arises near a solid boundary where the local Reynolds number becomes very small, resulting in laminar flow. This effect is built into the turbulence model by means of wall functions. These wall functions give a better description of the shear stresses near walls, resulting in more accurate values for *k* and for tangential velocities near a wall (Launder and Spalding 1974).

For airflow around the buildings, the no-slip condition cannot produce good results. Therefore, some types of artificial boundary conditions should be introduced to compensate for the effect of the viscous sub-layer.

In this study, $\frac{\partial \varepsilon}{\partial n} = 0$ should be set for the ground surface, whereas k = 0 can be set on that boundary.

For the ground surface and surfaces around the building blocks, excluding heating or pollutant sources, adiabatic and impermeable boundary conditions can be imposed, i.e., $\frac{\partial (T, \varphi_i)}{\partial n} = 0$.

Free stream boundaries (upper and side faces)

All the free stream boundaries are placed far enough from the buildings such that simplifying assumptions concerning these boundaries have so serious effects upon the flow inside the flow domain.

Three different ways can be adopted for free stream boundaries.

Firstly, scalars (k, ε, T, and φ_i) and tangential velocities can be described at the boundary, while no flow is allowed to cross the boundary. ($\boldsymbol{u}_\tau$ = constant, $\boldsymbol{u}_n$ = 0)

Secondly, flow can be prohibited from crossing the boundary, while zero gradient boundaries can be employed for tangential velocities and pressures. (эp/эn = 0, э$\boldsymbol{u}_\tau$/эn = 0, $\boldsymbol{u}_n$ = 0)

Thirdly, flow can be allowed to cross the boundary, while tangential velocities and pressures are prescribed. (p = constant, $\boldsymbol{u}_\tau$ = constant, э$\boldsymbol{u}_n$/эn = -э$\boldsymbol{u}_\tau$/эτ)

2.5 Convection visualization and heatfunctions

Streamfunction

The streamlines and heatlines are the best choice to visualize the paths followed by the fluid and heat flows [19, 30-35]. Such lines are defined, respectively, as the constant lines of the streamfunction (Ψ) and heatfunction (Θ). The dimensionless forms can be obtained,

$$\frac{\partial \psi}{\partial Y} = U \,, \quad \frac{\partial \psi}{\partial X} = -V \tag{33}$$

For fluid region

$$\frac{\partial \Theta}{\partial Y} = \mathrm{Re}\,\mathrm{Pr}\,U\theta - (1 + \mathrm{Re}\,\mathrm{Pr}\frac{C_\mu K^2 / E}{\sigma_t})\frac{\partial \theta}{\partial X}, \quad -\frac{\partial \Theta}{\partial X} = \mathrm{Re}\,\mathrm{Pr}\,V\theta - (1 + \mathrm{Re}\,\mathrm{Pr}\frac{C_\mu K^2 / E}{\sigma_t})\frac{\partial \theta}{\partial Y}$$

(34)

For solid region

$$\frac{\partial \Theta^*}{\partial Y} = -\mathrm{R_k}\frac{\partial \theta}{\partial X}, \frac{\partial \Theta^*}{\partial X} = -\mathrm{R_k}\frac{\partial \theta}{\partial Y} \quad (35)$$

The Ψ and Θ fields are defined through its first order derivatives, being thus important only differences in its values but not its level. This relative nature is similar to that of the pressure field in incompressible fluid flows. Thus, we have the freedom to state that,

$$\Psi(0, 0) = \Theta(0, 0) = 0 \quad (36)$$

As a heat transfer visualization technique, the use of heatlines is the convection counterpart or the generalization of a standard technique (heat-flux lines) used in heat conduction. If the fluid flow subsides (U = V = 0), the heatlines become identical to the heat-flux lines employed frequently in the study of conduction phenomena (Liu et al 2010).

$$\Theta = \Theta^*/k\triangle T, \quad (37)$$

2.6 Numerical methods

The equations described in the preceding section were solved numerically using the control volume formulation described by Patankar (1980). In the course of discretization, the third-order deferred correction QUICK scheme and second-order central difference scheme are, respectively, implemented for the convection and diffusion terms. The SIMPLE algorithm is chosen to numerically solve the governing differential equations in their primitive form. The steady momentum and energy equations were solved by a false unsteady scheme. For each time step, the discretized equations are solved by a line-by-line procedure, combining the tri-diagonal matrix algorithm (TDMA) and the successive over relaxation (SOR) iteration. It was assumed that the steady state was reached when the maximum local relative change in the velocity components and temperature was smaller than 10^{-6}; in addition, overall energy and mass balances $\oint_{\Gamma}(-\frac{\partial\Theta}{\partial X}+\frac{\partial\Theta}{\partial Y})dl=0, \oint_{\Gamma}(-\frac{\partial\Psi}{\partial X}+\frac{\partial\Psi}{\partial Y})dl=0$ less than 10^{-4} can determine the final steady fluid flow and heat transfer.

At $\tau \geq 0$ (upon that steady fluid flow and thermal convection have been achieved), the species transport Eq. (4) was solved iteratively. To obtain better convergence properties, the unsteady term in the equation is implicitly treated and hence approximated by backward differencing. The combined convection and diffusion terms are approximated by the power-law approximation. At each time step, the correspondent algebraic equation was invoked on a line-by-line basis using the TDMA algorithm. This process was repeated until the solution converged. The convergence criterion was a global one based on the relative incremental changes in the volume averaged pollutant concentration,

$$\frac{AC_{vol}^{N+1}-AC_{vol}^{N}}{AC_{vol}^{N}}<10^{-6} \qquad (38)$$

Admittedly, the pollutant will gradually emit from the cavity through the outlet with time elapse. Global conservation of pollutants pollutants cannot be checked on each time step due to this transient change. The reported results were obtained using the desktop, and the code was highly vectorized in order to reduce the CPU time, especially while solving the situations of higher Reynolds and Grashof numbers.

2.5. Grid independence, temporal step and code verification

The turbulence model has been validated by checking the results against those of benchmark solutions, where mixed convection in the slot vented enclosures has been tested numerically and experimentally (Papanicolaou and Jaluria, 1995; Costa et al 1999; Liu et al 2010).

Tests were conducted for all the applications to determine the dependency of solutions upon grid size. Solutions were obtained with successive refinement of grid size, i.e., reduction in the spacing between grid nodes in the *X* and *Y* directions. When solutions were observed to be unaffected by further refinements, they were presumed to be grid independent. Typically, for a 1:2 (H/W) enclosure at Re = 10^4 and Gr = 1010, 31×61, 41×81, 81×121, and 101×141 were tried, grid independence was achieved within 2.5% in Nu with a grid size of 81×121, and then the final grid resolution of 81×121 is selected at the balance between the calculation accuracy and the speed for mixed convection.

Temporal internal DT(Ds) is not fixed, but it is updated to asymptotically approach the real process, as illustrated in Fig. 2. Firstly, gaseous pollutants dispersed in the situation of Re = 2×10^3, Gr = 10^6 and Sc = 0.6, different steps DT = 0.1, 0.5, 1.0, 5.0 and 8.0 have been respectively applied for mixed ventilation mode (Fig. 2(a)), where remarkable average concentration differences of can be observed as pollutants initially emit from the source (s < 20) and these curves gradually approach that line of DT = 0.5

as time elapsed. Similarly, in terms of turbulent pollutant dispersions with displacement ventilation of Re = 10^4, Gr = 1010 and Sc = 0.6 (Fig. 2(b)), curves of large time step cannot disclose actual evolution of indoor pollutant emissions, particularly as emission time is less than 35. Therefore, smaller DT should be adopted to calculate the initial spread of indoor pollutants. DT= 0.1 was adopted in the present work.

The current numerical technique has been very successfully applied and validated in a series of recent papers, including laminar mixed convection [validation Zhao et al 2009, Liu et al 2012] and turbulent forced convection [Liu et al 2010] together with indoor pollutant emissions [Liu et al 2008].

3. Adjoint probability method for inverse identification of pollutant sources

Identifying pollutant sources according to measured pollutant concentrations is an inverse problem in that it is the problem of finding out unknown causes of known consequences. The adjoint probability method developed by Neupauer and Wilson (2001) for groundwater pollutant source identification, which can identify pollutant source location, flux and release time with little prior information, and the algorithm is faster than others. The method can be further used in indoor pollutant source identification. With a focus on identifying instantaneous point indoor pollutant sources, this paper presents the fundamentals of the CFD-based adjoint probability method and introduces the corresponding probability equations for different sensing scenarios.

We should introduce probability density function to explain the principles of the adjoint probability method. In a flow domain of interest, if a contaminant parcel is released from a point source at $\vec{x} = \overrightarrow{x_0}$ and $t = 0$, the forward location probability of the parcel is defined as the probability that it reaches some location in the domain at a given time $t = T > 0$. Assume the pollution source releases instantaneous contaminants with a mass of M_0 into the domain at $t = 0$, which spread all over the domain at t > 0 due to both convection and diffusion flows. If the pollutant mass trapped in a small finite volume ΔV_1 at $\vec{x} = \overrightarrow{x_1}$ at time $t = T$ is M_1, the forward location probability at this finite volume ΔV_1 at $t = T$ is

$$P(\Delta V_1 \left| \vec{x} = \overrightarrow{x_1}; t = T, \overrightarrow{x_0}) = \frac{M_1}{M_0} \right. \tag{39}$$

The location probability density function at $t = T$, is then defined as

$$f_x(\overrightarrow{x_1}; t = T, \overrightarrow{x_0}) = \frac{P(\Delta V_1 \left| \vec{x} = \overrightarrow{x_1}; t = T, \overrightarrow{x_0}) \right.}{\Delta V_1} = \frac{M_1}{M_0} \Big/ \Delta V_1 = \frac{C_1}{M_0} \tag{40}$$

where C_1 is the resident concentration at $\vec{x} = \overrightarrow{x_1}$, defined as a measure of the mass of pollutant per unit volume of flow medium, or a volume-averaged concentration. Generalizing the definition to all the locations in the domain yields,

$$f_x(\vec{x}; t = T, \overrightarrow{x_0}) = \frac{C(\vec{x}, T)}{M_0} \tag{41}$$

Where $f_x(\vec{x}; t = T, \overrightarrow{x_0})$ is the forward location probability density at $t = T$, $\vec{x}$ is the arbitrary location vector in the domain, $C(\vec{x}, T)$ is the distribution of resident pollutant concentration at t = T due to the instantaneous release of the point source, $\overrightarrow{x_0}$ is the given source location, M0 is the total source release mass. For the cases with steady-state velocity field, there is a linear relationship between source release strength and resident concentration, which leads to

$$f_x(\vec{x};t=T,\overrightarrow{x_0})=\frac{dC(\vec{x},T)}{dM_0}=\Psi_x(\vec{x};t=T,\overrightarrow{x_0}) \quad (42)$$

Where $\Psi_x(\vec{x};t=T,\overrightarrow{x_0})$ is the state sensitivity of resident concentration at $\vec{x}$ to the source M_0 at $\overrightarrow{x_0}$.

The forward location probability density function $f_x(\vec{x};t=T,\overrightarrow{x_0})$ describes the possibility of the pollutant parcel, originating from an instantaneous source at $\overrightarrow{x_0}$, to be at an arbitrary $\vec{x}$ after a fixed time t = T. From statistics, this forward location probability is equal to the possibility of the parcel found at $\vec{x}$ when t = T to be at source location $\overrightarrow{x_0}$ at t = 0 (or τ = T ago if a new backward time sign τ = T-t is defined), which is named as backward location probability $f_x(\vec{x}=\overrightarrow{x_0};t=T,\vec{x})$. The backward location probability can be determined via,

$$f_x(\vec{x}=\overrightarrow{x_0};t=T,\vec{x})=\Psi_x^*(\vec{x}=\overrightarrow{x_0};t=T,\vec{x}) \quad (43)$$

Where $\Psi_x^*(\vec{x}=\overrightarrow{x_0};t=T,\vec{x})$, termed as adjoint location probability, denotes the solution to an adjoint backward equation of the forward CFD pollutant transport equation.

The forward contaminant transport equation of CFD, can be expressed as equation (27).

The corresponding initial and boundary conditions are as follows,

$$C(\vec{x},0)=C_0(x) \quad (44)$$

$$C(\vec{x},0)=g_1(t) \text{ on } \Gamma_1 \quad (45)$$

$$\left[\upsilon_c\frac{\partial C}{\partial x_j}\right]n_j=g_2(t) \text{ on } \Gamma_2 \quad (46)$$

Where υ_c is the effective turbulent diffusion coefficient (usually scalar) for C. C_0 is the initial concentration, g_1, g_2, and g_3 are known functions, Γ_1, Γ_2 and Γ_3 are the domain boundaries, and n_i is the outward unit normal vector in the x_i direction.

The sensitivity analysis approach of Sykes et al. (1985) has been adopted to derive the adjoint backward equations from the forward pollutant transport equation (27). The corresponding CFD-based adjoint equation is shown as follows,

$$\left[\frac{\partial \Psi^*}{\partial \tau} - \frac{\partial V_j \Psi^*}{\partial x_j}\right] = \frac{\partial}{\partial x_j}\left[\upsilon_c \frac{\partial \Psi^*}{\partial x_j}\right] + (-q_O \cdot \Psi^*) + \frac{\partial h}{\partial C} \tag{47}$$

$$\Psi^*(\vec{x},0)=0 \tag{48}$$

$$\Psi^*(\vec{x},\tau)=0 \text{ on } \Gamma_1 \tag{49}$$

$$\left[\upsilon_c \frac{\partial \Psi^*}{\partial x_j} + V_j \Psi^*\right] n_j = g_2(t) \quad \text{on } \Gamma_2 \tag{50}$$

$$\frac{\partial h}{\partial C} = \delta(\vec{x} - \vec{x}_W) \cdot \delta(\tau) \tag{51}$$

For location probability

Where Ψ^* is the adjoint (location or travel time) probability, τ is the backward time, x_W is the location where the measurement is made, $\frac{\partial h}{\partial C}$ is the load term, and δ(x) is the impulse function which equals 1 when x = 0 otherwise 0. Note that the adjoint of the first type boundary condition is still first-type (boundary condition on Γ_1); the adjoint of the second-type boundary condition becomes third-type boundary condition onΓ_2. The initial condition $\Psi^*(\vec{x}, \tau=0) = 0$ implies that the adjoint probability for observed pollutants to be from any potential sources location is zero at the backward time τ=0. The boundary conditions restrain the adjoint probabilities at the boundaries. The load term represents a probability source term at the measurement point at τ=0.

To solve equation (47) requires information of air flow field, sensor location, boundary conditions, thermo-physical properties and geometric characteristics of the enclosed environment.

Adjoint probability method of inverse modeling deals with two basic concepts-location and travel-time probabilities. The development of this method includes three essential steps:

1. Understand the forward location and travel-time probabilities;
2. Establish the corresponding backward location and travel-time probabilities;
3. Derive the adjoint equations for the backward probability calculation from the forward governing equations.

4. Results and discussions

4.1 Steady fluid flow and conjugate heat and mass simulation

Firstly, Figure 3 presents the steady fluid flow and conjugate heat and mass transfer through mixed convection, displacement ventilation, mixed ventilation with top ceiling side (MVS) and displacement ventilation with left side (DVS). The air flow streamlines, isotherms, heat transport heatlines, turbulent kinetics and its viscosities (CuK2/E), under four categories of room ventilation schemes have been shown in Fig. 3, all with Re = 5×10^4, Gr = 10^8, Pr = 0.71, $\lambda S/\lambda F$ = 1.00. The computed streamlines, eddy viscosity, isotherms, iso-concentrations, and heatlines are plotted in the following figures, the intervals of these isopleths are $\Delta\Phi = (\Phi max-\Phi min)/16$, where Φ stands for variables in figures.

From the fluid flow streamlines, we can found that the external forced convection establishes the through flow from the left top vent to the right bottom vent for mixed ventilation (MV) in Fig. 3(a), whereas the counterclockwise flow eddy forms upon the carrying belt with the shear forces. With opposite effect of thermal buoyancy, thermal distribution was trapped on the bottom of the floor and does not extended to the upper zone. However, for mixed ventilation with top ceiling vent, the forced convection is with the aid effect of thermal buoyancy, the supplying jet can be extended to the right side and then ascending directly to the upper vent, as shown in Fig. 3(c). The co-rotating cellular of MV are with the same size and strength with MVS, even for the aid effect of thermal buoyancy forces and forced convection for MVS. As thermal buoyancy force is weak (low Grashof number), most of the turbulence for MV and MVS is originally generated near the outflow where stream flows impinge on the right upper wall (such as shown in Fig. 3(a) and (c)).

For the two displacement ventilation modes (DV and DVS), the outdoor fresh air flow into the room with the left bottom vent and flow out through the top right vent or top left vent as described in Figs. 3(b) and 3(d). Therefore, the forced convection and thermal buoyancy are both with aiding effect for DV and DVS. Multicellular flow patterns are presented due to solid blocks occurring. The general pattern of streamline is a flow route from the supply vent to the outlet, with two vortice embedded in the main cell on the surface of the bodies. Simultaneously, a secondary cell rotates clockwise at the central position of the floor due to the thermal buoyancy effect. The main vortice around the left solid block for DV mode decreases its size and moves to the lower part of the body, and is squeezed by the new counter-rotating cell around the body for the DVS mode.

Figure 5 presents the transient scenarios of pollutant concentrations under the aforementioned steady ventilation flow structures with the point pollutant source locating on S3 or S1, and all with the parameters of Qc/Qref = 1.00, Sc = 0.6, (ρD)S/(ρD)F = 1.00, ΔT = 1.00. Exposure to the contaminant may depend significantly on the contaminant source location. Here, we assume that slot-vented space is initially uncontaminated. When the flow injection begins, a net flow equal to the flow rate is established through the exit vent due to volume conservation. Subsequently, a pollutant source mentioned above is introduced to be located on S3 for MV and MVS or S1 for DV and DVS.

Originally, pollutant concentration is extracted from the source and transport within the room with the time going. For MV and MVS, the pollutant concentration in the lower space always tends to be lower than that of the upper air space. Ventilation mode makes an important role for pollutant diffusion. As expected, the pollutant always the highest one within this displacement ventilation space. Therefore, the concentration extraction process is exploiting the same mechanism as the fluid flow mechanism that makes these low energy systems so appealing compared with the other three ventilation modes. As seen in the constant concentration-line diagrams of Fig. 5, the solute intrusion flow moves forward along the floor, eventually forming stratified layers in this region, where the fluid moves very slowly along in the horizontal direction, enlarging with time and separating into a few rotate due to the obstacle blocks. Moreover, the continuous enlargement process of the concentration stratification is observed due to the accumulation of solutal source.

4.2 Probability Density Function (PDF) distributions for different pollutant source and sensor alarming

As the fluid flow distributions have been ‘measured’ when some sensor alarming at some temporal episode (such as $T^* = 50.0$), inverse modeling described in Section 3.0 will be implemented to identify the original pollutant source. The pollutant source has been identified through adjoint probability density function method. Different conditions have been in consideration, i.e., different pollutant source locations and different sensor alarming. Cases with only one sensor alarming have been calculated in the present work.

4.2.1 Central pollutant source identification with S1 or S3 as alarming sensor

Figure 6 indicates the spatial probability distributions for the central sensor SO with diverse ventilation arrangements and different sensor alarming time/pollutant traveling temporal probability, all with the parameters of $Sc = 0.6$, $(\rho D)S/(\rho D)F = 1.00$, $\Delta T^* = 1.0$. The final forward fluid flow simulation results are stored and treated as the exact fluid flow message as the initial fluid flow information for the spatial probability density function distribution computation. For MV and DV, S3 is alarming and PDF should be calculated. We can find for MV at T*=41 that the highest PDF is around the sensor location, where the most probability of pollutant source location. As time going back to T*=25, the highest PDF has transport to the boundary of green zone, where also has probability as pollutant source. When time goes to T*=10, the maximal PDF zone already move to the upper boundary of the solid block A. The PDF distribution changes a lot from T*=10 to T*=5 and even to T*=0. When T*=5, the highest PDF zone has been to over the right upper corner of the solid block A. Finally for T* approaching to zero, the highest PDF is at the central point of the vented room, which is the real pollutant source zone. Therefore, probability density function method has successfully identified the most probability pollutant source zone.

Ventilation mode made great importance on the PDF computation process. The conditions of the first and second columns are identical except the ventilation mode. The second column is under the displacement ventilation mode. S3 is alarming at T*=38, and the PDF distribution presents that the maximal PDF zone is at the left half ceiling position, not the S3 position under MV. The maximal PDF zone moves from the left upper corner to the left lower corner of solid block A during the period from T* = 25 to T*=5. When T* approaching to zero, the maximal PDF zone is at the central point and around lower part, which is the around upper part for MV mode.

The third and fourth columns present the S1 alarming under MVS and DVS modes. Due to the S1 position is under the solid block A, the original maximal PDF zone is at the S1 position under MVS mode. The movement of maximal PDF zone from the S1 position to the boundary of green zone when T*=10, and further to the left side of the vented room for T*=5. The maximal PDF distribution finally describes the maximal probability of pollutant source position is at the central position of the vented room. The spatial PDF distribution under DVS mode shows quite similar with that under MVS mode when T* greater than 10. When T*=5 under DVS, the maximal PDF zone is around the central of the left wall. The maximal PDF zone enlarges to the central for T*=2. The maximal PDF zone expresses the pollutant source at the central point.

4.2.2 Backward of probability distribution for different pollutant sources with different alarming sensors

As illustrated in Figs. 7–11, backward time simulation of probability density function (PDF) has been implemented in terms of different ventilation mode, different alarming sensor, and different pollutant source position, to identify pollutant sources on the floor. As shown in Fig. 7, temporal backward determination of pollutant source seems to be a bit difficult for DVS compared with other ventilation modes. This is due to the fact that sensitivity of pollutant dispersion has been inhibited at when pollutant source at outlet position. Actually, pollutant source at outlet makes most pollutant transporting to the outside and greatly confines pollutant dispersion and diminishes its sensitivities accordingly. Obviously illustrated in Figs. 8-11, identification of pollutant sources can be easily implemented for pollutant sources locating within the room, due to efficiently diffusion of pollutant concentration enhances the sensitivity of PDF backward time simulation.

However, with the backward time simulation of PDF, shown in Fig. 8, perturbation firstly occurs around the alarming sensor, and then the residuals of PDF asymptotically converge to the original position of pollutant sources.

Admittedly, different positions of pollutant sources will put effect on the inverse identification through probability density function distribution. Observing from Fig. 9, the pollutant sources will be easily identified for the concentrated pollutant strips, where pollutant diffusion is efficient comparing the pollutant source at outlet shown in Fig. 7. Similar results can also be found in Fig. 10-11 as thermal plumes become sensible and pollutant transportation become wide. As expected, the pollutant sources will be identified with a bit difficulty at the moment that the thermal buoyancy forces have put great effect on the pollutant spread. Therefore, identification of pollutant sources in large pitch and with thermal plume effects will be the most difficult situation.

5. Conclusions

The present work adopted the adjoint probability density function (PDF) method to identify of one contaminant source location with one sensor alarming in the ventilated enclosure with mixed and displacement ventilation flow patterns. The conclusions are as follows,

The definition and governing equation of probability density function (PDF) have been implemented. The history of Probability Density Function can be calculated for only one sensor alarming, with the steady-state airflow field, sensor location, boundary conditions, thermo-physical properties and geometric characteristics should be known in prior. Through the distribution of Probability Density Function nearly to T*=0, we can clearly identify the most possible location for the pollutant source. Probability Density Function (PDF) has been obtained for four types of ventilation modes and different sensor alarming. Different positions of pollutant sources will put effect on the inverse identification through probability density function distribution. The pollutant sources will be more easily identified for the concentrated pollutant strips, where pollutant diffusion is efficient comparing the pollutant source at outlet.

Overall, adjoint PDF methodology can be implemented well in the fields of natural gas leaking source identification, indoor air pollution control and building ventilation safety (to identify the terrorists' actions and report it timely), which puts great impact on the health of occupants in industrial society. Still, further researches, including the experimental rig system validation, noise data from the concentration sensors, and thermal plumes, will be investigated in the near future.

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